Author Index to Volume 8

Aboul-Seoud, A. See Sidrak, Y. L., 575
Aida, M. See Hosoya, H., 358
Allinger, N. L.
—; Lii, J.-H.: Benzene, Aromatic Rings, Van der Waals Molecules, and Crystals of Aromatic Molecules in Molecular Mechanics (MM3), 1146
—; Pathiaseril, A.: A Force Field for Allenes and for Nonlinear Acetylenes within the MM2 Approximation, 1225
—; See Liljefors, T., 1051
—; See Sprague, J. T, 581
Andzelm, J. See Radzio, E., 117

Bachrach, S. M. See Ritchie, J. P., 499
Back, D. M.
—; Polavarapu, P. L.: CNDO Force Constants for Glucose, 772
Baker, J.
An Algorithm for Geometry Optimization Without Analytical Gradients, 563
Bandrauk, A. D.
—; Gélinas, N.: Coupled Equations Approach to Multiphoton Molecular Processes, 313
Basilevsky, M. V.
—; Ryaboy, V. M.: Two Approaches to the Calculation of Molecular Resonance States: Solution of Scattering Equations and Matrix Diagonalization, 683
Bauschlicher, W., Jr.
—; Partridge, H.: Strategies for Vectorizing the Sparse Matrix Vector Product of CRAY XMP, CRAY 2, and CYBER 205, 636
Benard, M. See Laidlaw, W. G., 727
Bernardi, F.
—; McDouall, J. J. W.; Robb, M. A.: Transition Structure in a Diabatic Surface Formalism, 296
Bertrán, J. See Clavero, C., 481
Bertz, S. H. See Herndon, W. C., 367
Beveridge, B. L. See Jayaram, B., 917
Bickelhaupt, F. See Jenneskens, L. W., 1154
Billeter, M.
—; Havel, T. F.; Wüthrich, K.: The Ellipsoid Algorithm as a Method for the Determination of Polypeptide Conformations from Experimental Distance Constraints and Energy Minimization, 132
Bonaccorsi, R. See Pascual-Ahuir, J. L., 778
Boyd, R. J.
—; Edgecombe, K. E.: Bond Critical Points in the Electronic Structures of the Main Group Diatomic Hydrides of Lithium through Bromine, 489
Broyde, S. See Schlick, T., 1199
Brunvoll, J.
—; Cyvin, S. J.; Cyvin, B. N.: Enumeration and Classification of Benzenoid Hydrocarbons, 189
Bunge, C. F.
—; Cisneros, G.: Fast Matrix Multiplication, 960
—; See Cisneros, G., 618
Burggraf, L. W. See Stewart, J. J. P., 1117
Burke, L. A.
—; Kao, J.; Lilly, A. C., Jr.: Combination of MOMM and VEH Methods to Calculate Electronic Properties of Polymers, 107

Chirlian, L. E.
—; Francl, M. M.: Atomic Charges Derived from Electrostatic Potentials: A Detailed Study, 894
Cimiraglia, R.
—; Persico, M.: Recent Advances in Multireference Second Order Perturbation CI: The CIPSI Method Revisited, 39
Cioslowski, J.
Computer Enumeration of Polyhexes Using the Compact Naming Approach, 906
Cisneros, G.
—; Bunge, C. F.; Roothaan, C. C. J.: Fast Vector-Scalar-Multiply-and-Add Subroutines for VAX Computers, 618
—; See Bunge, C. F., 960
Clark, T. See Sptiznagel, G. W., 1109
Clavero, C.
—; Duran, M.; Lledós, A.; Ventura, O. N.; Bertrán, J.: Theoretical Study of the Addition of Hydrogen Halides to Olefins: A Comparison between $(HCl)_2$ and $(HF)_2$ Additions to Ethylene, 481
Clementi, E. See Kim, K. S., 57
—; See Largo-Cabrerizo, A., 1191
Contreras, R. H.
—; Gavarini, H. O.; Natiello, M. A.: The Through-Space Transmission of ^{77}Se-^{77}Se Coupling Constants, 265
Cremer, D.
—; Thiel, W.: On The Importance of Size-Consistency Corrections in Semiempirical MNDOC Calculations, 48
Crippen, G. M.
—; Ponnuswamy, P. K.: Determination of an Empirical Energy Function for Protein Conformational Analysis by Energy Embedding, 972
—; Voronoi Binding Site Models, 943
Cruickshank, D. W. J.
—; Eisenstein, M.: The Role of *d* Functions in AB-INITIO Calculations. II. The Deformation Densities of SO_2, NO_2, and Their Ions, 6
Cyvin, B. N. See Brunvoll, J., 189
Cyvin, S. J.
—; See Brunvoll, J., 189

Danaher, E. See Sanathanan, L., 1075
Datta, N. C.
—; Sen, B.: Recursion Formulae for Calculation of Overlap Integrals, 1
Davis, L. P. See Stewart, J. J. P., 1117
de Kanter, F. J. J. See Jenneskens, L. W., 1154
Demeter, D. A. See Lipkowitz, K. B., 753
de Wolf, W. H. See Jenneskens, L. W., 1154
Del Bene, J. E.
Basis Set and Correlation Effects on Computed Positive Ion Hydrogen Bond Energies of the Complexes $AH_n \cdot AH_{n+1}^{+1}$: $AH_n = NH_3$, OH_2, and FH, 810
Del Re, G. See Zuccarello, F., 816
Dillen, J. L. M.
On the Use of Constraints in Molecular Mechanics. II. The Lagrange Multiplier Method and Non-Full-Matrix Newton-Raphson Minimization, 1099
Dobbs, K. D.
—; Hehre, W. J.: Molecular Orbital Theory of the Properties of Inorganic and Organometallic Compounds. 5. Extended Basis Sets for First-Row Transition Metals, 861
—; Hehre, W. J.: Molecular Orbital Theory of the Properties of Inorganic and Organometallic Compounds. 6. Extended Basis Sets for Second-Row Transition Metals, 880

Duran, M. See Clavero, C., 481
Dutler, R. See Rauk, A., 324
Dykstra, C. E. See Loushin, S. K., 81

Edgecombe, K. E. See Boyd, R. J., 489
Edwards, W. D.
—; Weisman, G. R.: Quantum Mechanical Modeling of a Transannular Interaction in a Bicyclic Amidinium Ion, 149
Einstein, M. See Cruickshank, D. W. J., 6
El-Basil, S.
On Color Polynomials of Fibonacci Graphs, 956
Ezra, G. S. See Fried, L. E., 397

Fataftah, Z. A. See Ibrahim, M. R., 1131
Findley, G. L. See Georgian, T., 744
Forst, W. See Gidiotis, G., 420
Francl, M. M. See Chirlian, L. E., 894
Fraser, S. J.
Discrete Models of Growth and Dynamical Percolation in Chemistry, 428
Fried, L. E.
—; Ezra, G. S.: PERTURB: A Special-Purpose Algebraic Manipulation Program for Classical Perturbation Theory, 397
Fujita, T.
A Specific Inhibitor Design Approach by Means of Molecular Dynamics Calculation for Porcine Pancreatic Elastase, 645
—; Meyer, E. F., Jr.: Molecular Dynamics Simulation of the 1:1 Enzyme-Ligand Complex between Porcine Pancreatic Elastase and Acetyl-Alanine-Proline-Alanine, 801

Gavarini, H. O. See Contreras, R. H., 265
Gélinas, N. See Bandrauk, A. D., 313
Genest, M.
Theoretical Study of Water-Pyridine Complexes Using Intermolecular Potentials, 67
Georgian, T.
—; Halpin, J. M.; Findley, G. L.: Hamiltonian Dynamics of Chemical Reactions. Consecutive First-Order Reactions and Reactions Possessing One Autocatalytic Intermediate, 744
Gibson, K. D.
—; Scheraga, H. A.: Revised Algorithms for the Build-Up Procedure for Predicting Protein Conformations by Energy Minimization, 826
Gidiotis, G.
—; Forst, W.: Computational Aspects of Master Equation Transformation in Terms of Moments, 420
Gilliom, R. D.
—; Stoner, G. L.: Molecular Mechanics Study of Myelin Basic Protein, 1104
Glaser, R. See Streitweiser, A., Jr., 788
Glidewell, C.
—; Higgins, D.; Thomson, C.: An Investigation of the Relative Stabilities of the Isomers of CF_2N_2: Comparison of *ab initio* and MNDO Calculations, 1170
Go, N. See Wako, H., 625
Goddard, J. D.
Computational Studies of 1,2-Dithiete and Dithioglyoxal, 389
Goldblum, A.
Improvement of the Hydrogen Bonding Correction to MNDO for Calculations of Biochemical Interest, 835
Grigoras, S.
—; Lane, T. H.: *Ab Initio* Calculations on the Effect of Polarization Functions on Disiloxane, 84
Gropen, O.
Gaussian Basis Sets for the Fifth Row Elements, Mo-Cd, and the Sixth Row Elements W-RN, 982

Hafelinger, G.
—; Regelmann, C.: Refined ab initio 6-31G Split-Valence Basis Set Optimization of the Molecular Structures of Biphenyl in Twisted, Planar, and Perpendicular Conformations, 1057
Halpin, J. M. See Georgis, T., 744
Hambley, T. W.
Strain Energy Minimization Study of the Mechanism of, and the Barrier to, Conformational Interconversion in Five-Membered Diamine Chelate Rings, 651
Hariharan, P. C. See Kaufman, J. J., 736
Hässelbarth, W.
The Inverse Problem of Isomer Enumeration, 700
Havel, T. F. See Billeter, M., 132
Hehre, W. J. See Dobbs, K. D., 861
—; See Dobbs, K. D., 880
—; See Sptiznagel, G. W., 1109
Helman, A. J. See Lohr, L. L., 307
Helms, C. R. See Lopez, J. P., 198
Hemert, M. v. See Kaufman, J. J., 736
Herndon, W. C.
—; Bertz, S. H.: Linear Notations and Molecular Graph Similarity, 367
Hezemans, A. M. F. See Huige, C. J. M., 204
Higgins, D. See Glidewell, C., 1170
Hoffman, M. See Rössler, O. E., 510
Hopfinger, A. J. See Orchard, B. J., 28
Hosoya, H.
—; Aida, M.; Kumagai, R.; Watanabe, K.: Analysis of the π-Electronic Structure of Infinitely Large Networks. I. Some Remarks on the Characteristic Polynomial and Density of States of Large Polycyclic Aromatic Hydrocarbons, 358
—; See Randić, M., 522
Huige, C. J. M.
—; Hezemans, A. M. F.; Rasmussen, K.: Small Imines and Oximes as Model Compounds in the Optimization of a Consistent Force Field Potential Energy Function, 204
Huzinaga, S. See Sakai, Y., 226
—; See Sakai, Y., 256

Ibrahim, M. R.
—; Fataftah, Z. A.; Schleyer, P. v. R.; Stout, P. D.: Calculation of Enthalpies of Hydrogenation of Hydrocarbons, 1131
Iffert, R. See Jug, K., 1004
Iver, J. W., Jr. See McCourt, M., 454

Jayaram, B.
—; Mezei, M.; Beveridge, B. L.: Monte Carlo Study of the Aqueous Hydration of Dimethylphosphate Conformations, 917
Jenneskens, L. W.
—; de Kanter, F. J. J.; de Wolf, W. H.; Bickelhaupt, F.: MNDO Calculations on [n] Metacycylophanes, 1154
Jug, K.
—; Iffert, R.: Application of SINDO1 to Sulphur Compounds, 1004
—; Schulz, J.: Application of SINDO1 to Chlorine and Sodium Compounds, 1040
—; See Krüger, T., 350

Kaldor, U.
Open-Shell Coupled-Cluster Method: Electron Affinities of Li and Na*, 448
Kao, J. See Burke, L. A., 107
Karfunkel, H. R.
Molecular Mechanics and the Deformation of Macromolecules The Use of a Very Short Cutoff Combined with a Quadratic Approximation, 174
Kaufman, J. J.
—; Hariharan, P. C.; Roszak, S.; Hemert, M. v.: *Ab-Initio* MRD-CI Calculations of >A—NO_2 Decomposition Pathway of Nitrobenzene, 736
Kim, C. K. See Lee, I., 794
Kim, K.-H. See Sanathanan, L., 1075
Kim, K. S.
—; Clementi, E.: Hydration

Structures and Energetics of Phospholipid, 57
King, R. B.
Chemical Application of Topology and Group Theory. 23. A Comparison of Graph-Theoretical and Extended Hückel Methods for Study of Bonding in Octahedral and icosahedral Boranes, 341
Klein, D. J.
—; Randić, M.: Innate Degree of Freedom of a Graph, 516
Kleiner, A. F. See Randić, M., 522
Klobukowski, M. See Sakai, Y., 226
Klobukowski, M. See Sakai, Y., 256
Knop, J. V.
—; Müller, W. R.; Szymanski, K.; Kroto, H. W.; Trinajstić, N.: Computer Enumeration and Generation of Physical Trees, 549
—; See Müller, W. R., 170
Koehler, J. E. H.
—; Saenger, W.; Lesyng, B.: Cooperative Effects in Extended Hydrogen Bonded Systems Involving O—H Groups. *Ab Initio* Studies of the Cyclic S_4 Water Treatment, 1090
Kozmutza, C.
Ab Initio Program for Treatment of Related Molecules II. Integral Transformation in Extended Systems, 1179
Kramer, G. See Náray-Szabó, G., 555
Kroto, H. W. See Knop, J. V., 549
Krüger, T.
—; Jug, K.: Generalized Potential Surfaces under Inclusion of Nuclear Motion, 350
Kugler, S. See Náray-Szabó, G., 555
Kumagai, R. See Hosoya, H., 358

Laidlaw, W. G.
—; Benard, M.: Hartree Fock Instabilities of Sulfur-Nitrogen Systems: S_2N_2, 727
Laitenen, R. S.
—; Randolph, B.; Pakkanen, T. A.: Molecular Valence Calculations of Cyclohexasulfur, Cycloheptasulfur, and Cyclooctasulfur, 658
Landwer, J. M. See Lipkowitz, K. B., 753
Lane, T. H. See Grigoras, S., 84
Largo-Cabrerizo, A.
—; Clementi, E.: The Hylleraas-CI Method in Molecular Calculations: Two-Electron Integrals, 1191
Latajka, Z.
—; Scheiner, S.: Basis Sets for Molecular Interactions. 1. Construction and Tests on $(HF)_2$ and $(H_2O)_2$, 663
—; Scheiner, S.: Basis Sets for Molecular Interactions. 2. Applcation to $H_3N—HF$, $H_3N—HOH$, $H_2O—HF$, $(NH_3)_2$, and $H_3CH—OH_2$
Lee, B. C. See Lee, I., 794
Lee, I.
—; Kim, C. K.; Lee, B. C.: Theoretical Studies on the Acid Hydrolysis of Methyl Carbamate, 794
Lesyng, B. See Koehler, J. E. H., 1090
Lewis, D. F. V.
Molecular Orbital Calculations on Solvents and Other Small Molecules: Correlation between Electronic and Molecular Properties μ, $\alpha_{MCL, and \beta}$, 1084
Li, S. See Liljefors, T., 1051
Lii, J.-H. See Allinger, N. L., 1146
Liljefors, T. See Pettersson, I., 1139
—; Tai, J. C.; Li, S.; Allinger, N. L.: On the Out-of-Plane Deformation of Aromatic Rings, and Its Representation by Molecular Mechanics, 1051
Lilly, A. C., Jr. See Burke, L. A., 107
Liotard, D.
—; Roche, M.: Topology of Conical Intersections and Jahn-Teller Crossing: Application to the Standard Model for XY_4 Molecules in T_2 Ground States, 850
Lipkowitz, K. B.
—; Demeter, D. A.; Parish, C. A.; Landwer, J. M.: Column Design. 3. Theoretical Studies of a Chiral Stationary Phase Used in Column Chromatography, 753
Lipson, J. E. G.
Simulation Studies of Branched Polymer Molecules, 333
Lledós, A. See Clavero, C., 481
Lohr, L. L.
—; Helman, A. J.: Centrifugal Distortions in Molecules: An Ab Initio Approach with Application to Ozone, 307
Lopez, J. P.
—; Yang, C. Y.; Helms, C. R.: Electronic Structure of Clusters Modeling Silica, 198
Loushin, S. K.
—; Dykstra, C. E.: Polarization Counterpoise Corrections to Correlated Hydrogen Bond Interaction Energies, 81

March, N. H.
The Density Amplitude ρ^{112} and the Potential which Generates It, 375
Martin, Y. See Sanathanan, L., 1075
Matias, M.
—; Tel, L. M.; Novoa, J. J.: *Ab Initio* Studies on Van Der Waals Molecules. A Comparative Study with Several Basis Sets of the *C2v* HeLi2 System, 51
—; Varandas, A. J. C.: *Ab Initio* Study of the $He(^1S)$-$Li_2(X,^1E_g^+)$ Interaction by the SCF and MP2 Methods, 761
McCourt, M.
—; Iver, J. W., Jr.: On the SCF Calculation of Excited States: Singlet States in the Two-Electron Problem, 454
McDowell, R. S. See Streitweiser, A., Jr., 788
McDuall, J. J. W. See Bernardi, F., 296
Meyer, E. F., Jr. See Fujita, T., 801
Mezei, M. See Jayaram, B., 917
Mezey, P. G.
Introduction, 281
—; The Shape of Molecular Charge Distributions: Group Theory without Symmetry, 462
Millet, K. C.
Stereotopological Indices for a Family of Chemical Graphs, 536
Miyoshi, E. See Sakai, Y., 226
Miyoshi, E.
—; See Sakai, Y., 256
Müller, W. R. See Knop, J. V., 549
Müller, W. R.
—; Szymanski, K.; Knop, J. V.; Trinajstić, N.: An Algorithm for Construction of the Molecular Distance Matrix, 170
Murcko, M. A. See Wiberg, K. B., 1124

Nagy, P. See Náray-Szabó, G., 555
Náray-Szabó, G.
—; Kramer, G.; Nagy, P.; Kugler, S.: Towards a Quantum Chemical Software Package Utilizing Transferable Fragments as Molecular Building Blocks, 555
Natiello, M. A. See Contreras, R. H., 265
Neuberger, J. W.
—; Noid, D. W.: Numerical Calculation of Eigenvalues for the Schrödinger Equation. III, 459
Niño, A. See Smeyers, Y. G., 380
Noid, D. W. See Neuberger, J. W., 459
Novoa, J. J. See Matias, M., 51

Ojha, R. P. See Sanyal, N. K., 272
Orchard, B. J.
—; Tripathy, S. K.; Pearlstein, R. A.; Hopfinger, A. J.: Molecular Modeling of Polymers: I. Correct and Efficient Enumeration of Intrachain Conformational Energetics, 28
Overton, M. See Schlick, T., 1025
—; See Schlick, T., 1199

Pakkanen, T. A. See Laitenen, R. S., 658
Parish, C. A. See Lipkowitz, 753
Pascual-Ahuir, J. L.
—; Silla, E.; Tomasi, J.; Bonaccorsi, R.: Electrostatic Interaction of Solute with a Continuum. Improved Description of the Cavity and of the Surface Cavity Bound Charge Distribution, 778

Pathiaseril, A. See Allinger, N. L., 1225
Patil, N. See Rothstein, S. M., 412
Partridge, H. See Bauschlicher, W., Jr., 636
Pearlstein, R. A. See Orchard, B. J., 28
Persico, M. See Cimiraglia, R., 39
Peskin, C. See Schlick, T., 1199
Pettersson, I.
—; Liljefors, T.: Benzene-Benzene(Phenyl-Phenyl) Interactions in MM2/MMP2 Molecular Mechanics Calculations, 1139
Poirier, R. A.
—; Surján, P. R.: The Application of Strictly Localized Geminals to the Description of Chemical Bonds, 436
Polavarapu, P. L. See Back, D. M., 772
Ponder, J. W.
—; Richards, F. M.: An Efficient Newton-like Method for Molecular Mechanics Energy Minimization of Large Molecules, 1016
Ponnuswamy, P. K. See Crippen, G. M., 972

Radzio, E.
—; Andzelm, J.: Reliable Gaussian Basis Sets for Closed-Shell Atoms, 117
Randić, M. See Klein, D. J., 516
—; Woodworth, W. L.; Kleiner, A. F.; Hosoya, H.: Graph Generators, 522
Randolph, B. See Laitenen, R. S., 658
Rasmussen, K. See Huige, C. J. M., 204
Rauk, A.
—; Dutler, R.: Implementation and Applications of Gaussian 82 on a CDC Cyber 205, 324
Regelmann, C. See Hafelinger, G., 1057
Richards, F. M. See Ponder, J. W., 1016
Ritchie, J. P.
—; Bachrach, S. M.: Some Methods and Applications of Electron Density Distribution Analysis, 499
Robb, M. A. See Bernardi, F., 296
Roche, M. See Liotard, D., 850
Roothaan, C. C. J. See Cisneros, G., 618
Rössler, O. E.
—; Hoffman, M.: Quasiperiodization in Classical Hyperchaos, 510
Roszak, S. See Kaufman, J. J., 736
Rothstein, S. M.
—; Patil, N.; Vrbik, J.: Time Step Error in Diffusion Monte Carlo Simulations: An Empirical Study, 412
Rouvray, D. H.
The Modeling of Chemical Phenomena Using Topological Indices, 470
Roychoudhury, M. See Sanyal, N. K., 272
—; See Sanyal, N. K., 604
Ruelle, P.
Theoretical Study on the Mechanism of the Thermal Decarboxylation of Acrylic and Benzoic Acids. Models for Aqueous Solution, 158
Ruhela, K. R. See Sanyal, N. K., 604
Ryaboy, V. M. See Basilevsky, M. V., 683

Saenger, W. See Koehler, J. E. H., 1090
Sakai, Y.
—; Miyoshi, E.; Klobukowski, M.; Huzinaga, S.: Model Potentials for Molecular Calculations. I. The *sd*-MP Set for Transition Metal Atoms Sc through Hg, 226
Sakai, Y.
—; Miyoshi, E.; Klobukowski, M.; Huzinaga, S.: Model Potentials for Molecular Calculations. II. The *spd*-MP Set for Transition Metal Atoms Sc through Hg, 256
Sanathanan, L.
—; Danaher, E.; Kim, K.-H.; Martin, Y.: Systematic Drug Receptor Mapping: A New Approach to the Analysis of Conformational Energy Calculations of Flexible Molecules with Application to Dopaminergic and Adrenergic Agonists, 1075
Sanyal, N. K.
—; Ojha, R. P.; Roychoudhury, M.: Interaction Energy Studies of 8-Azapurine during Transcription, 272
—; Roychoudhury, M.; Ruhela, K. R.; Tivari, S. N.: Configurational Specificity of Stacking Interactions in DNA Base Pairs: A Computational Analysis, 604
Scheiner, S. See Latajka, Z., 663
—; See Latajka, Z., 674
Scheraga, H. A. See Gibson, K. D., 826
Schleyer, P. v. R. See Ibrahim, M. R., 1131
—; See Spitznagel, G. W., 1109
Schlick, T.
—; Overton, M.: A Powerful Truncated Newton Method for Potential Energy Minimization, 1025
—; Peskin, C.; Broyde, S.; Overton, M.: An Analysis of the Structural and Energetic Properties of Deozyribose by Potential Energy Methods, 1199
Schulz, J. See Jug, K., 1040
Schwenke, D. W.
—; Truhlar, D. G.: Converged Calculations of Rotational Energy Transfer in HF—HF Collisions, 282
Sen, B. See Datta, N. C., 1
Senn, P.
A Note on the Efficient and Accurate Computation of the Phase Functions ϕ and χ in Semiclassical Approximations, 965
Sidrak, Y. L.
—; Aboul-Seoud, A.: An Objective Computer-Oriented Method for the Calculation of Formation Constants from the Formation Function. A Weighted Least-Squares Curve Fitting, 575
Silla, E. See Pascual-Ahuir, J. L., 778
Simon, J.
Molecular Graphs as Topological Objects in Space, 718
Smeyers, Y. G.
—; Niño, A.: Character Tables and Symmetry Eigenvectors for Two C_{3v} Rotor Molecular Systems, 380
Spitznagel, G. W.
—; Clark, T.; Schleyer, P. v. R.; Hehre, W. J.: An Evaluation of the Performance of Diffuse Function-Augmented Basis Sets for Second Row Elements, Na-Cl, 1109
Sprague, J. T.
—; Tai, J. C.; Yuh, Y.; Allinger, N. L.: The MMP2 Calculational Method, 581
Stewart, J. J. P.
—; Davis, L. P.; Burggraf, L. W.: Semi-Empirical Calculations of Molecular Trajectories: Method and Applications to Some Simple Molecular Systems, 1117
Stoner, G. L. See Gilliom, R. D., 1104
Stout, P. D. See Ibrahim, M. R., 1131
Streitweiser, A., Jr.
—; McDowell, R. S.; Glaser, R.: A Study of Basis Set Effects on Structures and Electronic Structures of Phosphine Oxide and Fluorophosphine Oxide, 788
Surján, P. R. See Poirier, R. A., 436
Szöke, J.
Optimized Method for the Evaluation of the Convolutionally Distorted Decay Curves, 95
Szymanski, K. See Knop, J. V., 549
—; See Müller, W. R., 170

Tai, J. C. See Liljefors, T., 1051
—; See Sprague, J. T., 581
Taylor, K. F.
On Madelung's Constant, 291
Tel, L. M. See Matias, M., 51
Thiel, W. See Cremer, D., 48
Thomson, C. See Glidewell, C., 1170
Tivari, S. N. See Sanyal, N. K., 604

Tomasi, J. See Pascual-Ahuir, J. L., 778
Topiol, S.
Comparison of the Use of the MNDO and MINDO/3 Methods with *Ab Initio* Methods to Study Tautomerism in Histamine, 2- and 4-Methylhistamine, 142
Trinajstić, N. See Knop, J. V., 549
—; See Müller, W. R., 170
Trindle, C.
Application of the NuMATH Computer Algebra System to Sets of First Order Kinetic Equations of Significance in Chemistry, 442
Tripathy, S. K. See Orchard, B. J., 28
Truhlar, D. G. See Schwenke, D. W., 282

Varandas, A. J. C. See Matias, M. A., 761
Ventura, O. N. See Clavero, C., 481
Vrbik, J. See Rothstein, S. M., 412

Wako, H.
—; Go, N.: Algorithm for Rapid Calculation of Hessian of Conformational Energy Function of Proteins by Supercomputer, 625
Watanabe, K. See Hosoya, H., 358
Weisman, G. R. See Edwards, W. D., 149
Wiberg, K. B.
—; Murcko, M. A.: Nonbonded Interactions. 1. Anistropic Hydrogen-Hydrogen Interactions, 1124
Woodworth, W. L. See Randić, M., 522
Wüthrich, K. See Billeter, M., 132

Yang, C. Y. See Lopez, J. P., 198
Yuh, Y. See Sprague, J. T., 581

Zuccarello, F.
—; Del Re, G.: Towards a Valence-Orbital/Bond-Orbital Description of Biochemical H-Bonds from *Ab Initio* Calculations, 816

Subject Index to Volume 8

Ab initio calculations, basis sets for, 663, 674, 982
Ab initio calculations, comparison with MNDO and MINDO/3 on histamine tautomerism, 142
Ab initio calculations, *d* functions in, 6
Ab initio calculations, for atomic charges, 894
Ab initio calculations, for geometry optimization without analytical gradients, 563
Ab initio calculations, the Hylleraas-CI method in, 1191
Ab initio calculations, in hydrogen bonds in water, 1090
Ab initio calculations, integral transformations in, 1179
Ab initio calculations, the localized geminal description of bonds, 436
Ab initio calculations, model potentials for transition metal atons, 226, 256
Ab initio calculations, of bond critical points in electronic structures of the main group diatomic hydrides, 489
Ab initio calculations, of chemical reactions, 296
Ab initio calculations, of enthalpies of hydrogenation, 1131
Ab initio calculations, of He-Li_2 interaction, 761
Ab initio calculations, of hydrogen bond energies, 810
Ab initio calculations, of hydrogen bonding, 81
Ab initio calculations, of multiphoton molecular processes, 313
Ab initio calculations, of orbitals in hydrogen bonds, 816
Ab initio calculations, of the thermal decarboxylation of acrylic and benzoic acids, 158
Ab initio calculations, on the addition of hydrogen halides to olefins, 481
Ab initio calculations, on biphenyl, 1057
Ab initio calculations, on CF_2N_2, 1170
Ab initio calculations, on complexes of small molecules, 674
Ab initio calculations, on cyclosulfur compounds, 658
Ab initio calculations, on disiloxane, 84
Ab initio calculations, on 1,2-dithiete, 389
Ab initio calculations, on dithioglyoxal, 389
Ab initio calculations, on excited states, 454
Ab initio calculations, on first-row transition metals, 861
Ab initio calculations, on ozone, 307
Ab initio calculations, on phosphine oxide and fluorophosphine oxide, 788
Ab initio calculations, on phospholipid hydration, 57
Ab initio calculations, on S_2N_2, 727
Ab initio calculations, on SO_2, NO_2, and their ions, 6
Ab initio calculations, on transition metals, 861, 880
Ab initio calculations, on van der Waals molecules, 51
Ab initio calculations, on water dimer, and HF dimer, 663
Ab initio calculations, open-shell, coupled-cluster method, 448
Ab initio calculations, with Gaussian 82 on a Cyber 205, 324
Ab initio (MRD-CI) calculations, nitrobenzene, 736
Acrylic acid, thermal decarboxylation, by *ab initio* calculations, 158
Adrenergic agonists, molecular mechanics calculations on, 1075
Alkenes, addition of hydrogen halides to, by *ab initio* calculations, 481
Allenes, molecular mechanics calculations on, 1225
Altmann groups for C_{3v} rotors, 380
Aromatic hydrocarbons, cyclic and linear polymers of, 358
Autocatalytic reactions, kinetics of, 744
8-Azapurine, interaction energy studies of, 272

Basis sets, for *ab initio* calculations, 663, 674, 982
Basis sets, Gaussian, for closed-shell atoms, 117
Benzene-benzene interactions, in molecular mechanics calculations, 1139, 1146
Benzenoid hydrocarbons, enumeration and classification, 189
Benzoic acid, thermal decarboxylation, by *ab initio* calculations, 158
Biphenyl, *ab initio* calculations on, 1057
Bond critical points, in main group diatomic hydrides, by *ab initio* calculations, 489
Boranes, a comparison of graph-theoretical and extended Hückel methods for, 341

Centrifugal distortions on molecules, 307
Charge distribution, some methods and applications of, 499
Charge distributions, shapes of, 462
Charge interactions, of a solute with a continuum, 778
Charges, derived from electrostatic potentials, 894
CNDO calculations, on glucose, 772
Color polynomials of Fibonacci graphs, 956
Configuration Interaction by Perturbation, 39
Configuration interaction, size-consistency corrections in, 48
Conformational analyses, of polymers, 28
Conical intersections and Jahn–Teller crossing, 850
Coupled-cluster method, in *ab initio* calculations, 448
CRAY, vectorizing the sparse matrix vector product on, 636
CYBER 205, vectorizing the sparse matrix vector product on, 636
Cyclosulfur compounds, *ab initio* calculations on, 658

Density amplitude $\rho^{1/2}$, 375
Deoxyribose, molecular mechanics calculations on, 1199
Diabatic surface model on chemical reactions, 296
Dimethylphosphate, Monte Carlo calculations on hydration of, 917
Disiloxane, *ab initio* calculations on, 84
Distance matrix, molecular, algorithm for construction of, 170
Distorted delay curves, evaluation of, 95
1,2-Dithiete, *ab initio* calculations on, 389
Dithioglyoxal, *ab initio* calculations on, 389
Dopaminergic agonists, molecular mechanics calculations on, 1075
Dragt–Finn perturbation theory, 397

Effective core potentials, for atoms Sc through Hg, 226, 256
Eigenvalues by numerical calculations, 459
Elastase, pancreatic, molecular dynamics calculation on, 645
Electron affinities, of Li and Na, 448
Electrostatic interactions, of a solute with a continuum, 778
Electrostatic potentials, charges from, 894
Energy embedding, for protein structure, 972

Energy minimization, in molecular mechanics, 1016, 1025
Energy transfer, in thermal systems, calculation of, 420
Enzyme inhibitor design, by molecular dynamics, 645
Enzyme-ligand complex, molecular dynamics calculations on, 801
Excited states, SCF calculation, 454
Extended Hückel calculations on boranes, 341

Fano–Feshbach theory of resonance, 683
Fibonacci graphs, color polynomials of, 956
Formation constants, calculation of, 575

Gaussian basis sets, for closed-shell atoms, 117
Gaussian 82, implementation on a Cyber 205, 324
Geminals, localized, for bond description in *ab initio* calculations, 436
Geometry optimization, *ab initio*, without analytical gradients, 563
Glucose, CNDO force constants for, 772
Graph generators, 522
Graph, innate degree of freedom of, 516
Graph theory, applied to boranes, 341
Graphs, generation of physical trees, 549
Graphs, highly symmetrical vertex transitive, 522
Graphs, stereotopological indices for, 536
Group theory and C_{3v} rotor systems, 380
Group theory, without symmetry, 462
Growth and dynamical percolation, models of, 428

Heats of hydrogenation, *ab initio* calculations of, 1131
HF——HF collisions, rotational energy transfer in, 282
Histamine tautomerism, by *ab initio*, MNDO, and MINDO/3 calculations, 142
Hydrogen bond energies, *ab initio* calculations on, 810
Hydrogen bonding, *ab initio* calculations of, 81
Hydrogen bonding, between water and pyridine, 67
Hydrogen bonding, in MNDO calculations, 835
Hydrogen bonds, *ab initio* description of, 816
Hydrogen bonds, in water, *ab initio* calculations on, 1090
Hylleraas-CI method in *ab initio* calculations, 1191
Hyperchaos, classical, quasiperiodization in, 510

Imines, molecular mechanics calculations on, 204
INDO calculations, on a bicyclic amidinium ion, 149
Isomer enumeration, inverse problem of, 700

Jahn–Teller crossing and conical intersections, 850

Kinetic equations, first order MuMATH computer algebra system, solution of, 442
Kinetics, consecutive first-order reactions and reactions possessing one autocatalytic intermediate, 744

Lagrange multiplier method, 1099
Least squares method, nonlinear, 95
Lie transform algorithms, 397
Linear notation systems, for molecular graphs, 367

Madelung's constant, 291
Matrix multiplication, fast, 960
Meiron method, 95
Metacyclophanes, MNDO calculations on, 1154
Methyl carbamate hydrolysis, MNDO calculations on, 794
MINDO calculations, of electronic and molecular properties, 1084
MNDO calculations, for reaction trajectories, 1117
MNDO calculations, hydrogen bonding correction in, 835
MNDO calculations, on CF_2N_2, 1170
MNDO calculations, on the hydrolysis of methyl carbamate, 794
MNDO calculations, on metacyclophanes, 1154
MNDO and MINDO/3 calculations, comparison with *ab initio* methods in histamine, 142
MNDOC calculations, size-consistency in, 48
Modeling, using topological indices, 470
Model potentials, atoms Sc through Hg, 226, 256
Molecular dynamics calculations, of the enzyme-ligand complex, 801
Molecular dynamics calculations, for enzyme inhibitor, 645
Molecular graphs, as topological objects, 718
Molecular graphs, for linear notations, 367
Molecular mechanics calculations, benzene-benzene interactions in, 1139, 1146
Molecular mechanics calculations, nonbonded potentials in, 1124
Molecular mechanics calculations, of chiral recognition in column chromatography, 753
Molecular mechanics calculations, of protein conformations, 826
Molecular mechanics calculations, on aromatic rings, 1051
Molecular mechanics calculations, (MMP2) on conjugated systems, 581
Molecular mechanics calculations, on conformational interconversion in five-membered diamine chelate rings, 651
Molecular mechanics calculations, on deoxyribose, 1199
Molecular mechanics calculations, on imines and oximines, 204
Molecular mechanics calculations, on macromolecules, cutoff approximation, 174
Molecular mechanics calculations, on myelin protein, 1104
Molecular mechanics calculations, on nonlinear acetylenes, 1225
Molecular mechanics, calculations, on receptor mapping, 1075
Molecular mechanics, calculations, on water and pyridine, 67
Molecular mechanics, energy minimization in, 1016, 1025
Molecular mechanics, energy minimization methods in, 1099
Molecular mechanics, for polypeptides, 132
Molecular mechanics, molecular orbital based (MOMM), 107
Monte Carlo calculations, on dimethylphosphate hydration, 917
Monte Carlo calculations, on phospholipid hydration, 57
Monte Carlo calculations, on polymers, 333
Monte Carlo simulations, diffusion time step error in, 412
Multiphoton molecular processes, *ab initio* calculations of, 313
Myelin protein, molecular mechanics calculations on, 1104

Newton–Raphson minimization, 1099
Nitrobenzene decomposition, *ab initio* calculations of, 736
Nonbonded potentials, for H_2/H_2 interactions, 1124
Nonlinear acetylenes, 1225
Nucleic acids, stacking interactions in, 604
Numerical calculations, of eigenvalues, 459

Out-of-plane deformations, of aromatic rings, molecular mechanics calculations on, 1051
Overlap integrals, recursion formulae for calculation of, 1
Oximines, molecular mechanics calculations on, 204
Ozone, centrifugal distortions of, 307

Perfluorodiazirine, calculations on, 1170
Perfluorodiazomethane, calculations on, 1170
Perturbation configuration interaction, 39
Perturbation theory, special-purpose algebraic manipulation program for, 397
Phase functions, computation of, 965

Phosphine oxide, *ab initio* calculations on, 788
Phospholipids, hydration structures and energetics of, 57
Polarization functions, effect on disiloxane calculations, 84
Polyhexes, enumeration of, 906
Polymer molecules, Monte Carlo calculations on, 333
Polymers, electronic properties of, by molecular mechanics calculations, 107
Polymers, molecular modeling, 28
Polypeptide conformations, from experimental distance constraints and energy minimization, 132
Polystyrene, conformational analysis of, 28
Potential surfaces, with inclusion of nuclear motion, 350
Protein conformations, by molecular mechanics calculations, 826
Protein structure, by energy embedding, 972
Protein structure, from molecular mechanics calculations, 1104
Proteins, molecular mechanics calculations on, cutoff approximation, 174
Proteins, rapid calculations of the Hessian energy functions of, by supercomputer, 625
Pyridine-water complexes, molecular mechanics calculations on, 67

Reaction dynamics, by MNDO calculations, 1117
Reactions, *ab initio* calculations of, 296
Receptor mapping, 1075
Receptors, geometries from substrates, 943
Resonance states, molecular calculation of, 683
Rotational energy transfer, on HF——HF collisions, 282

Semi-empirical calculations, on glucose, 772
Semi-empirical calculations, of Se——Se coupling constants, 265
Semi-empirical calculations, on 8-azapurine during transcription, 272
Semi-empirical calculations, on boranes, 341
Semi-empirical calculations (SINDO1), on chlorine and sodium compounds, 1004
Semi-empirical calculations, on silica, 198
Semi-empirical calculations, on structure stacking interactions in DNA, 604
Semi-empirical calculations (SINDO1), on sulphur compounds, 1040
Semi-empirical calculations, see MNDO, MINDO, etc.
Semi-empirical calculations, utilizing transferable fragments, 555
Se——Se coupling constants, 265
Siegert–Humblet–Rosenfeld theory of resonance, 683
Silica, electronic structure, 198
Sulphur compounds, semi-empirical calculations on, 1040
Supercomputers, Gaussian 82 on, 324
Supercomputers, rapid calculation of the Hessian of the energy function by, 625
Supercomputers, vectorizing the sparse matrix vector product on, 636

Topological indices, modeling in, 470
Transannular interaction, by INDO calculations, 149
Transition metal atoms Sc through Hg, model potential method on, 226, 256
Transition metals, *ab initio* calculations on, 861, 880

van der Waals molecules, *ab initio* calculations on, 51
Van Vleck perturbation theory, 397
VAX computers, subroutine for scalar-multiply-and-add operations, 618
Vectorizing the sparse matrix vector product, on supercomputers, 636
Vector-scalar-multiply-and-add subroutines for VAX computers, 618
Vibronic Schrödinger equation, solution of, 350
Voronoi binding site models, 943

Water, *ab initio* calculations on hydrogen bonding in, 1090
Water dimer, *ab initio* calculations on, 663
Water-pyridine complexes, molecular mechanics calculations on, 67